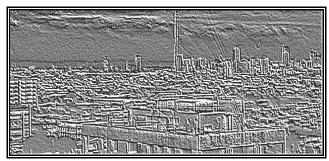
### "World Water Crisis Predicted as Cities Continue to Grow"

"The scarcity of water is replacing oil as a flashpoint for conflict between nations in an increasingly urbanized world .....With most of mankind poised to live in cities in the next millennium, the world must brace for a 'water shock' as wrenching as the "oil shock" of the 1970's, panelists told the "Water for Thirsty Cities" forum."

—Chicago Tribune, May 7, 1996.

"Mankind's future will unfold largely in urban settings."

—Mega-City Growth and the Future Fuchs et al., United Nations University Press, 1994



### **URBAN SECURITY**

### ANNUAL REPORT FOR FISCAL YEAR 1997

LOS ALAMOS NATIONAL LABORATORY LOS ALAMOS, NEW MEXICO

"The urban research agenda for the 1990's should focus on the identification of innovative approaches to deal with complex issues in urban management and on strengthening national capacities to plan and implement urban development programs"

—G. S. Cheema, in Mega-City Growth and the Future

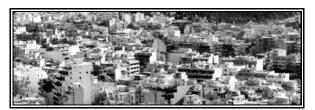
### "Mass weapons threat deepens worldwide"

"The deepening threat...is the terrorist use of nuclear, biological, and chemical weapons to inflict mass urban casualties and social paralysis almost anywhere in the world."

—Aviation Week and Space Technology, June 17, 1996.

### Why Should The Los Alamos National Laboratory Study Urban Systems?

It is widely recognized that short- and longterm national security depends upon a judicious balance of investment in defense, economic, social, educational, and environmental programs. The vitality of our national infrastructure, which overlaps and merges with the aforementioned programs, is therefore critical to our national security. We contend that our nation is most vulnerable where the infrastructure elements converge in cities. United Nations-sponsored studies point to a great need to focus on the vulnerability of cities around the world that are experiencing explosive growth. Mega-City Growth and the Future (edited by Fuchs et al., United Nations University Press, 1994) opens with the following statement that motivates this proposal: "Mankind's future will unfold largely in urban settings."



### Our vision for the Los Alamos National Laboratory is to:

Develop a cross-divisional applied research competency to model the response and vulnerability of urban systems to changes in physical environment, malicious attacks, socio-political setting, and the economy.

To understand urban systems demands multidisciplinary approaches that account for physical processes, economic and social factors, and nonlinear feedback across a broad range of scales and disparate process phenomena. Strong research programs in the defense, environmental, and computational arenas at the Laboratory have developed many state-of-the-art models that will serve as components of an urban modeling system. These include programs in transportation, air quality, groundwater transport, energy

distribution, network theory, communications, synthetic population modeling, natural hazards, and risk assessment. We are building on these and other modeling tools, modifying them for urban settings, and linking them together as an integrated simulation system that takes advantage of our high performance computing (HPC) platforms. We are engaging collaborators from the urban planning community and university campuses to ensure relevance and to eliminate "wheel reinventing."

The Los Alamos National Laboratory's vision is to be "a national laboratory in which science serves society to enhance global security, preserve the earth, and improve the quality of life through innovations in science and technology..." In order to remain a major locus of research leading to global stabilization, we are working to understand urban systems and their vulnerabilities. Integrated urban systems research is right for the Laboratory because it will maintain our ability to integrate across disciplines, requires great science, and maintains the Laboratory as a national resource through multi-agency sponsorship. Urban systems research will directly strengthen three core competencies that, in turn, support the core Laboratory mission—Earth & Environmental Systems; Analysis & Assessment; and Theory, Modeling & High Performance Computing.

Interest from the government in addressing urban systems issues will, by necessity, grow over the next several years. Such growth is already indicated in DOE by the following: (1) creation in 1996 of a new program to address biological/chemical terrorism in cities; (2) establishment in 1996 of the DOE Center of Excellence for Sustainable Development; (3) plans for creation of the DOE Center of Excellence for Disaster Response in 1997. The range of agencies that have, or will have, a stake in components of urban systems includes DOE, DOD, DOT, EPA, HUD, FEMA, UN, state and local planning agencies, and corporate sponsors.

# Accomplishments of the 1997 Urban Security Pilot Project

The work during fiscal year 1997 focused in an effort titled "Urban Security—A High-Performance Computing Pilot Project.' During this year we have engaged a team representing five Laboratory divisions and a range of expertise including atmospheric and hydrologic modeling, software design, mathematics, geographic information systems (GIS), geology, and urban planning. One major part of the pilot project was to link regional atmospheric modeling with ground water models in order to assess vulnerability of urban water supplies to climate change. Another part of the pilot project was to model the transport of an airborne toxic gas, including effects of buildings on air flow, and to link this to traffic simulations for effective emergency response. Other activities were to establish connections with potential collaborators and funding agencies, as well as highlighting the project through presentations at professional meetings.

# The Effects of Global Change on the Albuquerque Water Supply (coupled atmospheric and hydrologic models)

The Río Grande provides an essential water supply for the flora, fauna, and human population along its course through Colorado, New Mexico, and the Texas/Mexico border. The headwaters of the Río Grande, in the San Juan Mountains, southern Colorado, are fed primarily by snowmelt from winter storms. In contrast, the lower portions of the river receive runoff from thunderstorms of the summer monsoon. Thus, the waters of the Rio Grande are strongly influenced by regional climate and could be vulnerable to climate change. Albuquerque's water supply may be affected by changes in regional climate as manifested by variation in Río Grande water levels. We rely on the use of coupled atmospheric, runoff, and ground water models. Preliminary work in 1997 focused on uncoupled simulations of the aquifer beneath Albuquerque and winter precipitation simulations of the upper Rio Grande basin.

To examine the temporal variability, simulations were carried out with the Regional Atmospheric Modeling System (RAMS), at 20-km² resolution, for the months of January, 1996 (a representative dry extreme) and January 1993 (a representative wet extreme). A case study has been developed for one particular storm at higher resolution (5 km²) over the Río Grande headwaters to examine spatial variability of the snowpack within complex terrain.

In support of the water supply portion of the 1997 urban securities CD Thrust, a mapbased interactive graphical tool has been developed for analysis and comparison of model output and surface weather station data.

The map exists as a metafile which can be displayed on an X-Window computer using the utility 'idt'. It consists of a contour map of topography of the Rio Grande drainage (most of Colorado and New Mexico) with the COOP and SNOTEL stations located on it (Fig. 1). Using the mouse and the zoom capability of "idt", the user can delimit a certain area of the map and pass those delimiting coordinates to a process running in another window. This process then produces, for example, time series line plots, in a separate window, of precipitation for each station within the area chosen. Also, model precipitation (interpolated to station locations within this area), or the difference between model output and station data can also be plotted. Alternatively, stations within the specified area can be averaged and plotted vs. other averaged areas chosen by the user. For instance, line plots of precipitation over the Jemez Mountains can be compared to that over the southern San Juan Mountains and northern Sangre de Cristo Mountains through some time period of interest. Again, model output can be included in the plots or not as the user sees fit.

Another type of plot is produced by the corco module. The plot consists of the same contour map of topography onto which is plotted (located), for example, all stations whose time series of a requested variable

correlates well (say correlation coefficient > 0.9) with a station chosen (using mouse and zoom) from the original map with all stations. All parameters are input by the user on-the-fly. The time this or any module takes to produce a plot is < 4 sec. This allows the user to graphically peruse the data and/or model results looking for subtleties such as orographically-induced effects.

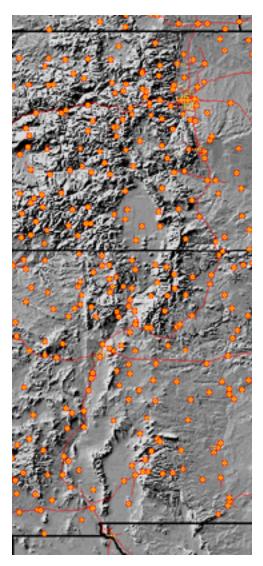


Fig. 1. Surface weather stations used in modeling regional climate effects on he Río Grande watershed, and ultimately, the Albuquerque water supply. This section of the image covers the upper Río Grande Basin across Colorado and New Mexico

Future plans will be to add stream flow data to the map interface. This should be valuable in verification of the surface hydrology model as well as looking at correlations between temperature increases at higher elevations and stream flow increases at lower elevations. A standard deviation module similar to the corco module might be useful. For instance, all stations having standard deviation within 10% of a chosen station could be plotted. Adding modules for other types of analyses is easily done.

Finally, moving this tool to a Geographic Information System (GIS) environment, as long as the interactivity is maintained could certainly enhance its usefulness.

This component of Urban Security will be primarily associated with the Coupled Environmental Modeling CD thrust in 1998.

#### Airborne Toxic Response/Emergency Response

If a tanker truck carrying hazardous chemicals overturns in a city, could emergency response crews estimate the exposure to vehicles that unwittingly drove through the poisonous cloud? Or, if a terrorist releases a chemical or biological agent in the downtown area, could first responders figure out how the toxic agent spread, where it ended up, and how much was transported away from the scene by moving vehicles? Research now underway at Los Alamos National Laboratory as part of the Urban Security Project might help emergency response personnel answer some of these questions.

The goal of the Airborne Toxic Response/ Emergency Response task was to demonstrate a capability for analyzing emergency response issues resulting from accidental or meditated airborne toxic releases in an urban setting. In the first year of the program, we linked a system of fluid dynamics and vehicle transportation models developed at Los Alamos to study the dispersion of a plume in an urban setting and the resulting exposures to vehicle traffic (see fig. 2).

The HOTMAC prognostic mesoscale model computed three-dimensional meteorological fields over a domain of several hundred

kilometers. Zooming in to higher resolution using a nested grid computational mesh, the wind and turbulence fields computed on a 2 km grid size provided boundary conditions for a higher resolution simulation of flow around two 2-d buildings using the GASFLOW computational fluid dynamics code.

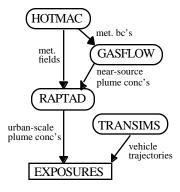


Figure 2. Flowchart showing the links between the mesoscale atmospheric model HOTMAC, the microscale fluid dynamics model GASFLOW, the Lagrangian dispersion model RAPTAD, and the TRANSIMS traffic simulation model.

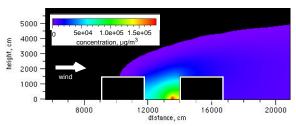


Figure 3. Concentration field computed by the GASFLOW model for a surface release in an urban canyon.

A gas source was located at ground level between the two buildings and the near-source transport and dispersion of the contaminant cloud was simulated at several meter resolution using the GASFLOW model (Fig. 3). Due to recirculation and trapping between the two buildings, concentrations are highly elevated there. The cloud is also lofted very high into the atmosphere downstream of the buildings, a condition of the enhanced turbulent mixing resulting from the building obstructions.

This has an important impact once the plume is passed from the microscale GASFLOW domain to the mesoscale HOTMAC/RAPTAD domain. The pollutant cloud travels farther downwind in a given amount of time when the effects of buildings are explicitly accounted for (Fig. 4). Although buildings

act to slow down the flow by imparting drag, the lofting of the plume in this particular case results in the cloud being carried by the higher wind speeds aloft. A paper entitled "The effect of microscale urban canyon flow on mesoscale puff dispersion" attached in the Appendix gives more detail on this portion of the research.

A simulation performed by the TRANSIMS team computed traffic flow for over 100,000 vehicles in North Dallas. TRANSIMS represents a new approach in traffic modeling where the movement of individual cars is performed using cellular automata techniques. The interaction of the cars on the microscale results in macroscopic traffic patterns seen in common



Figure 4. Comparison of GLC fields computed a) with the HOTMAC-RAPTAD and GASFLOW modeling systems and b) with the HOTMAC-RAPTAD modeling system only. This figure shows that explicit modeling of buildings significantly impacts plume transport and dispersion.

everyday traffic. Figure 5 depicts the major roadways in the vicinity of the plume, along with the intersection nodes in the simulated domain.

Vehicle trajectory and plume concentration data were used to compute exposures to over 36,000 vehicles traveling through the timevarying contaminant cloud in the Dallas-Ft. Worth area (Figure 6). The agent is transported by the vehicles over a much larger area than that covered by the plume (Fig. 7). Moreover, the final locations of vehicles with high exposure is not intuitively obvious.

Using a modeling system like this, emergency response personnel could determine the impact zones, the optimal routes for response teams, where casualties might occur, and how the agent is dispersed. The efforts of clean-up crews and medical teams could be enhanced as well with knowledge of the final location and levels of exposure. Further research efforts are underway at Los Alamos to better estimate the impact of multiple buildings on plume transport and dispersion. Research on transportation simulation continues at LANL, including efforts to abstract the fundamental vehicle flow dynamics so that problems can be run on PC platforms.



Figure 5. Major roadways impacted by the the contaminant cloud. Diamonds represent intersection nodes and cover the entire active simulation region.

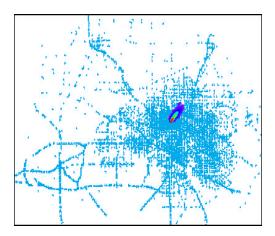


Figure 6. Node locations of the roadway network in the Dallas-Ft. Worth area. The spatial extent of the plume location 10 minutes after release is depicted. The red box demarcates the region of active traffic simulation.

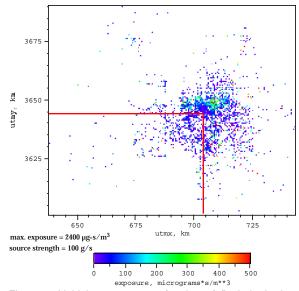


Figure 7. Vehicle exposure as function of final destination. Intersection of red lines denote contaminant plume source location. The dimensions of the roadway network in fig. 5 match those here.

### Summary of 1997 Results

Already we are seeing the following tangible results of the pilot project: (1) papers on water supply issues in a rapidly growing "sunbelt" city and on air contaminant transport in an urban environment accepted for presentation in international conferences; (2) existing atmospheric, hydrologic, and GIS capabilities successfully stretched to new regimes for urban applications; (3) design criteria established for implementation of coupled models on the ASCI HPC platform; (4) team members appointed to the Megacities Committee of the International Union of Geodesy and Geophysics (IUGG); we proposed to the IUGG and to the International Union of Geological Sciences (IUGS) that the years 2001-2010 be declared the "Decade of the City," in which the geological and geophysical sciences be focused on urban problems and the response was very positive; (5) Collaborations are being developed with the UCLA (School of Public Health, Institute of the Environment) and Arizona State University (Dept. of Mechanical and Aerospace Engineering); (6) building a collaboration with the DOE Center for Excellence for Sustainable Development and with academic urban simulation experts;

and (7) building a collaboration with the Southern California Earthquake Center.

# Our Approach to Modeling Urban Systems (1998-1999)

Urban systems are composed of a wide range of subsystems: transportation, construction, energy distribution, communication systems, ground- and sub-surface water transport, air transport and fate, geology, ecosystem, solid waste, food and water distribution, economic zones, and demographics, for example. We are linking the many components of an urban system, rooting our framework in sophisticated high fidelity physics models and abstracting the essential physics, social, and economic interactions so that decision-makers can answer questions of importance on urban security (see Fig. 8). We are modeling the physics of these subsystems in detail using state-of-the-art models developed within the Laboratory. A challenging aspect of this research effort is the physics of the interfaces

between the models (right hand side, Fig. 8). These subsystems are linked and their interaction produces the collective and often non-intuitive behavior of the urban system. This part of the framework demands high performance computing (HPC) since each subsystem alone can be an HPC-scale problem.

Our approach is to emphasize linking cross-disciplinary subsystem models, tailoring them for urban applications, and writing interface physics modules. We are accomplishing this with a portfolio of research topics that force tailoring and interfacing of the subsystem models. Our early efforts focus on the high-level/low-level interface (middle, Fig. 8), then shift toward decision-making tools (left hand side, Fig. 8).

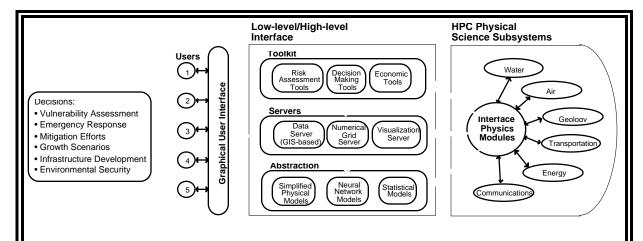


Figure 8. Schematic of proposed system architecture for answering urban security questions. Sophisticated numerical models from across disciplines and covering a broad range of scales will be integrated through interface physics modules. Methods for abstracting the "essential" physics will be utilized to speed computations and generalize results. Links between the physics-based models will be made to decision-making tools. Servers will provide data and visualization tools to the end-user.

Examples of Integrated Cross-Disciplinary Subsystem Models: As examples of needed urban modeling problems, we have chosen two problems that cover a broad range of urban subsystems and

that have pressing real-world applications. Many of the modeling tools mentioned below exist at Los Alamos for national security and weapons complex applications, and others must be developed. The linked, complex systems approach will bring these tools into a new realm of applications, allow us to answer previously unresolvable problems, and at the same time will sharpen and maintain our ability to use them for future security and environmental problems.

#### Transportation-Air-Water Systems

The transport and fate of nitrates in the urban environment has important health and global climate implications, involves many of the urban subsystems, and the physics of the complete cycle is not understood. The following subsystems and their interfaces will be brought into the urban system framework: traffic simulation; mesoscale atmospheric processes; building-scale computational fluid dynamics and dispersion; air pollution chemistry; deposition and resuspension physics; and urban surface water, ground water, and river discharge transport and chemistry (see Fig. 9). We emphasize

that this example of a linked system of models could be applied to most any air- and water-borne contaminant.

We follow the nitrates from their beginning as nitrate-precursors produced by auto emissions and industrial processes, track their dispersion and chemistry as they swirl around buildings and eventually deposit on the ground in patterns that are determined by the micro-meteorology and surface characteristics. Intermittent gusts caused by winds or passing vehicles can subsequently re-suspend the deposited particulates and deposit them in new locations. Much of the

deposited material is entrained into surface water runoff during rain events, and then carried into sewers, natural water- ways, and groundwater where dispersion and chemical reactions take place. Nitrates in the water supply can have serious health effects on children and nitrates discharged to the ocean can upset the ecosystem balance and contribute to global climate change.

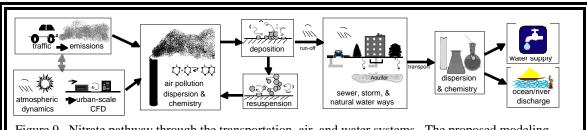


Figure 9. Nitrate pathway through the transportation, air, and water systems. The proposed modeling system can be applied to many different kinds of air contaminants (e.g., from accidental spills, industrial sources, a CBW attack). The air/water modules could be used in reverse to track vapors emanating from underground sources, as in many EM clean-up projects.

To succeed in this research challenge, there must be development of interface physics modules linking different types of Laboratory models. For example,

TRANSIMS, a model for simulating the travel behavior of individuals in a city and a TRANSIMS emissions sub-model that translates second-by-second vehicle

attributes into spatial and temporal distributions of automobile emissions will be interacting with a linked system of fluid dynamics models composed of the GASFLOW, HIGRAD, and RAMS models. The fluid dynamics models would capture phenomena from weather to buildings scales, i.e., from hundreds of kilometers down to meters, a problem that requires HPC platforms. Feedback

between modeling systems exist that have not adequately been modeled in the past. For example, inclement weather reduces traffic flow, stop-and-go traffic increases tail-pipe emissions, emissions are

affected by temperature, and traffic disperses emissions. Although smallscale plume chemistry can be simulated by an innovative Lagrangian dispersion

model called RAPBOX, detailed deposition and re-suspension physics of particulates are poorly understood.

Accurate simulation of building-scale fluid dynamics, vehicle-induced wakes and turbulent transport will be key to development in this area. Rain events modeled using the RAMS mesoscale atmospheric code will lead to urban surface runoff into storm, sewer, and natural waterways. FEHM-GEOMESH, a sophisticated numerical package for groundwater flow and chemistry, will be used to determine the fate of the nitrates once in the soils. New interface modules are needed to adequately couple the physics of very different systems, atmospheric/near-surface conditions and surface/subsurface infiltration. The standard surface, storm, and sewer water transport models used in the public works engineering community will be improved in house. This type of research will result in substantial new science and will be, to our knowledge, the first full life cycle model of a pollutant such as the nitrates.

### Infrastructure Damage from Natural Disasters

Natural disasters such as earthquakes severely stress the urban infrastructure system and can be a major test of our understanding of how infrastructure elements are linked. Such stresses have been clearly demonstrated at Northridge (California, 1994), Kobe (Japan, 1995), and Mexico City (1985). A primary cause of the damage in these events is attributed to complex geologic structures such as sedimentary basins, which amplify and prolong ground motion. The HPC

platform being implemented in the Laboratory ASCI program, for example, would be an excellent platform on which to perform simulations of the necessary size and resolution (order 10<sup>7</sup>-10<sup>8</sup> finite difference cells) to accurately predict ground motion patterns. We are developing nonlinear modules that will enable existing elastic codes to better predict ground motion in areas of high vulnerability. The combination of unprecedented problem size, resolution, and nonlinear wave propagation will be a major step forward in seismic risk modeling.

In parallel with adaptation of the earthquake simulation codes, damage modules must be linked to a modeled pattern of ground motions, which can be projected into specific predictions of damage to urban subsystems and to critical parts of the infrastructure. For example, downed communications will adversely affect the electrical power system, transportation, and food and goods distribution, and these feed back into effects on general recovery efforts. This modeling framework will then be useful for emergency response and sustainable development planning, infrastructure and economic warfare vulnerability assessment, and a range of natural disaster scenarios beyond earthquakes.

Los Alamos is co-hosting a workshop on "Earthquakes and Urban Infrastructure" with the Southern California Earthquake Center in Los Angeles in January 1998. the purpose is to have infrastructure organizations such as CalTrans supply input about their needs linking modeling of ground motion witn infrastructure damage, emergency response, and recovery, with the goal of using the models for urban infrastructure planning.

# Design of the Low-level Framework (Subsystems Interface Physics) Server

A large part of the power of an urban system modeling framework resides in

the interface physics module. This module will link subsystems models to the extent necessary, which in some cases may involve full coupling. Because of the physical problem size and the number of unknown variables, a subset of the individual models will require access to the high speed parallel machines. These models will, in turn, depend upon a data server for input and output in a common GIS format, and on a grid server that supports parallel implementations. The numerical grid server will support decomposition algorithms for time dependent calculations, and the visualization server will provide levels of visualization appropriate for a varied user base. We will select a development platform that is multithreaded. distributed, object-oriented, and has a rich set of predefined class libraries. This strategy will minimize the amount of effort devoted to server implementation and maximize the resources available to the interface module and to the subsystems models.

### Abstraction Modeling Efforts

One very challenging aspect of this research is how to interface the low-level, computer-intensive, physics-based models to the end-user in a computationally efficient and straightforward manner. Laboratory teams would use simpler physics-based models, neural networks, adjoint operator methods, and/or statistical models to bridge the gap between the end-user and low-level models. Simpler physics-based models will be derived or existing models improved, based on subsystem modeling results. In this way, simplifying assumptions and parameterizations inherent in the high-level models can be tested. Neural nets, adaptive learning systems that mathematically develop relationships between data sets, will be designed from large data sets produced by the physics-based models. Neural nets use no physics, only statistical relationships. The advantage of this method is that it is very fast and easy to use; the disadvantage is that when

conditions change, the statistical relationships, based on old data, are no longer valid. Uncertainties in model results, clearly needed for decision-making tasks, will be ascertained using statistical models on data produced by the low-level physics models or by using adjoint operator methods.

### Tool Kit/Graphical User Interface (GUI) Development

A relevant problem that links a simple physics-based model with economic and risk assessment tools is the development of a graphical user interface, database and visualization servers, the end-user tool kit, and linking abstraction models with decision-making tools. We must understand the feedback mechanisms between decision-making tools and science models.

#### Validation and Case Studies

Validation must occur at all model levels, including interface physics models, subsystem models, damage modules, and the total system decision tool. No one city will provide the necessary infrastructure database and Geographic Information System (GIS) to satisfy the validation needs of the full urban system framework. We are seeking a pragmatic approach to validation, taking advantage of established projects with a well developed city database and GIS.

- The 1997 pilot project is currently adapting to an already established transportation modeling effort in North Dallas to develop and validate aspects of the transportation and atmospheric process interface.
- Similarly, part of the pilot project is studying water resources in Albuquerque because the data from recent studies provide an excellent base for comparison with model results.

For infrastructure damage from natural disasters, we may be working with the Southern California Earthquake Consortium to model seismic response and infrastructure weaknesses in the Los Angeles Basin; this study will provide validation because of the well-characterized geology, excellent geophysical monitoring, and infrastructure data.

 We have a collaboration with scientists from the Unversidad Nacional Autonoma de Mexico, to determine effects of a volcanic ash fallout on the infrastructure of Mexico City.

Furthermore, an obvious link with the LANL Remote Sensing project can provide unique information obtained from satellite platforms and ground-based instruments. Validation of the developing urban system framework and high-level decision tools will play a major role in distinguishing Los Alamos' Urban Security Competency from urban planning research elsewhere.

### Cooperation With Other Competency Development Projects at Los Alamos

#### **Coupled Environmental Modeling**

There is considerable overlap between the goals of the Coupled Environmental Modeling project and Urban Security. There will be considerable sharing of HPC tools and technical staff. The major difference is one of scale.

#### **Remote Sensing**

The potential collaboration between the Remote Sensing Initiative and Urban Security is significant. In many cases, up-to-date comprehensive observational data are not available for many cities—Urban Security needs those data. Staff for the Remote Sensing Initiative are actively developing next generation sensors, which could be used to observe

cities, producing data ranging from comprehensive observations of topography and structures to vegetation health as a sustainability indicator.

# Cooperation with Ongoing Programs at Los Alamos

- TRANSIMS (Transportation Simulation)
- Seismic Risk evaluation
- Mexico City air quality
- Yucca Mountain hydrologic modeling
- Hydrologic modeling for the Environmental Restoration Program
- Environmental studies
- Nuclear, Biological, and Chemical threats
- Infrastructure assurance analysis
- Environmental security

## Collaborators and Potential Collaborators

Donald Duke, UCLA—Environmental Science and Engineering, School of Public Health

Renato Funiciello. Universita di Roma-III

Tom Henyey, Directory, Southern California Earthquake Center (USC)

Patrick Lana, DoE—Center of Excellence for Sustainable Development

Luis Marin, Universidad Autonoma de Mexico (UNAM)—Instituto de Geofisica Kim Olsen, UCSB—Institute of Crustal Studies

Giovanni Orsi, Universita di Napoli

W. Ostercamp, US Geological Survey, Earth Surface Processes, Materials Use, and Urban Development (ESPROMUD)

Ray Punongbayan, Philippine Institute of Volcanology and Seismology (Manila)

Claus Siebe, UNAM—Instituto de Geofisica

Uri Shamir, Israel Inst. Technology (water and megacities)

Ken Snyder, DoE—Center of Excellence for Sustainable Development

Irene Tinker, UCB—Institute of Urban and Regional Planning

Rich Turco, UCLA—Environmental Institute

Roger White, Memorial University, St. Johns, Newfoundland

Lyna Wiggins, Rutgers University— Center for Urban Policy Research

# Post-Doctoral Fellows and Students (GRA)

This part of the project is being developed, especially through University of California campuses.

The first Post-Doctoral Fellow is James Stalker, from the University of Alabama—Huntsville, who is working with Costigan and Bossert on atmospheric modeling.

# **Key Project Personnel at Los Alamos**

Jim Bossert: EES-8. Ph.D., Atmospheric Science. Areas of interest: Mesoscale and microscale atmospheric modeling, regional climate modeling, fire weather modeling, urban plume dispersion. bossert@lanl.gov

Michael Brown: TSA-4. Ph.D. Atmospheric Sciences. Areas of Interest: Turbulence, Boundary-layer, Plume Dispersion, Urban Canyon, and Mesoscale Meteorological Modeling. brown@viento.lanl.gov Julie Canepa: EM-ER. Ph.D., Chemistry. Disposition of nuclear waste in geologic media, environmental geochemistry, complex system integration, and urban security. canepa\_julie@lanl.gov

Keeley Costigan: EES-5. PhD., Atmospheric Sciences. Areas of Interest: Numerical simulation with the Regional Atmospheric Modeling System (RAMS) and analysis of complex terrain meteorology, including flow in valleys and air quality studies. Numerical simulation of the large eddies of the atmospheric boundary layer and their interaction with larger scale circulation. krc@vega.lanl.gov

Jonathan Dowell: TSA-4, Ph.D., Engineering Physics. Areas of interest: power-systems engineering, graph theory, GIS/GUI development. Developed analysis algorithms and interfaces for the Infrastructure-Assurance Analysis Project (IAAP), including Power-System and Natural-Gas/Petroleum-Pipeline Analyzers. ljdowell@lanl.gov

Denise George: T-1. MS, Computer Sciences. Areas of Interest: Software System Design, Parallel and Distributed Computing.

Wayne Hardie: TSA-4. M.A, Nuclear Engineering. Areas of Interest: Energy and environmental analysis and modeling. hardie@lanl.gov

Grant Heiken: EES-1. Ph.D., Geology. Areas of Interest: Natural hazards, applied volcanology, urban geology. heiken@lanl.gov

Eric Jones: EES-5. Ph.D., Astronomy. Areas of Interest: Seismology, numerical modeling, space. Laboratory Fellow. honais@lanl.gov

David Langley: EES-8. B.S. Mathematics; Graphics, atmospheric processes. dll@lanl.gov.

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George Niederauer: TSA-10. Ph.D., Nuclear Engineering, Areas of Interest: Computational fluid mechanics, porous media and aerosol modeling, nuclear facility containment issues. gfn@lanl.gov

Barbara Sinkule: CST-7. Ph.D., Civil Engineering—Specializing in environmental engineering and water resources planning. Areas of interest: Water resources and environmental planning; hazardous waste and radioactive waste projects. sinkule@lanl.gov

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La Ron Smith: TSA-DO/SA. PhD. Nuclear Engineering. Areas of Interest: complex systems, risk management, transportation simulation. llsmith@lanl.gov

Jake Turin: CST-7. Ph.D., Hydrology. Areas of Interest: Vadose-zone hydrology, subsurface contaminant transport, groundwater geochemistry, and karst hydrology. turin@lanl.gov

Greg Valentine: EES-5. Ph.D., Geology. Areas of Interest: Transport processes in geologic media, plumes, convection, magma dynamics, flow in porous media, explosive volcanism, high-speed multiphase flows, computational fluid dynamics, hydrothermal systems, planetary processes. gav@vega.lanl.gov

Mike Williams: TSA-4. Ph.D., Mechanical and Nuclear Engineering. Areas of Interest: Emissions modeling, plume chemistry modeling, air quality, and meteorological modeling. mdw@lanl.gov

# **Invited Speakers at Urban Security Team Meetings**

Charryl Berger, Los Alamos National Laboratory, Industrial Partnership Office, "What is the potential industrial interest in urban security?"

Don Duke, UCLA-Environmental Health Sciences, "Industrial pollutants and environmental health in a large metropolis"

Wolfgang Eder, Director, Earth Sciences, UNESCO, "UNESCO cities program"

Paul Gilna, OHER lab representative for Los Alamos National Laboratory, "Mission of the DOE Office of Health and Environmental Research"

Ray Gordon, Los Alamos National Laboratory, TSA-4, "Infrastructure Assurance"

Carl Hagelberg, Los Alamos National Laboratory, EES-5, "Modeling and prediction of epidemic systems in an urban setting"

Wayne Hardie, Los Alamos National Laboratory, TSA-4, "National economic system simulation" Dennis Hjeresen, Los Alamos National Laboratory, EM-DO, "Environmental Security"

Patrick Lana, DOE-Center of Excellence for Sustainable Development, discussion of the Center's national program

Tom Meyer, Los Alamos National Laboratory, DOD-PO, "Shaping 21st Century Warfare" Darrell Morgeson, Los Alamos National Laboratory, TSA-DO, "National Security and National Infrastructure"

Randy Mynard, Los Alamos National Laboratory, EES-15, "DOD/FEMA emergency preparedness coordination"

George Niederauer, Los Alamos National Laboratory TSA-10, "GASFLOW"

Waite Osterkamp, US Geological Survey, "Earth Surface Processes, Materials Use, and Urban Development (ESPROMUD)"

Claus Siebe, Universidad Nacional Autonoma de Mexico, "Natural hazards in Mexico City"

Ron Smith, Los Alamos National Laboratory TSA-DO, "TRANSIMS"

Paul Weber, Los Alamos National Laboratory, NIS-2, "Remote sensing initiative and possible links to urban security"

Tom Wehner, Los Alamos National Laboratory, TSA-3, "Overview of Government programs concerning NBC"

Lyna Wiggins, Center for Urban Policy Research, Rutgers University, "Urban GIS and Links to Modeling"

### **Description of Models**

FEHM (Finite Element Heat and Mass transport code) solves the equations of multiphase, multi-component fluid flow and species transport, along with heat transport, in porous and/or fractured media. It uses a finite element approach and is used for a wide variety of applications including vadose zone hydrology, reactive transport of dissolved species and radionuclides, saturated zone hydrology, geothermal reservoir modeling, and petroleum reservoir models.

**GASFLOW** - a three dimensional computational fluid dynamics model used

primarily for solving building interior and exterior flow fields. Solves the compressible Navier-Stokes equations using the ICED-ALE finite difference scheme. Turbulence represented by k-e closure. Resolution of flow fields typically about a meter. Unique features include combustion of flammable gases, chemical reaction mechanisms, entrainment and deposition of aerosols.

GEOMESH is part of a family of codes that generate unstructured meshes for finite difference and finite element models. GEOMESH is especially tailored for precise representation of complex geologic media in three dimensions, including discontinuous beds, faults, and folds, with little if any grid artifacts. It is currently used to build finite element meshes primarily for FEHM flow and transport simulations.

**HOTMAC** (Higher Order Turbulence Model for Atmospheric Circulation) - a prognostic three-dimensional mesoscale atmospheric model used for computing meteorological flow fields in complex terrain. Solves the incompressible hydrostatic geophysical equations using the ADI finite difference scheme. Turbulence represented by the k-l closure. Horizontal resolution typically about 1 kilometer and vertical resolution about 4 meters near the surface and expanding with height. Accounts for land class variations, urban and forest canopy effects, and has nested grid and data assimilation capabilities.

RAPTAD (Random Particle Transport And Diffusion) - a Lagrangian random-walk puff dispersion model used to compute concentration fields in complex terrain. Uses meteorological fields produced by HOTMAC as input. Thousands of pollutant puffs are released one after another, transported by the mean wind and spread by the turbulent field. Accounts for buoyant plume rise, point, area, and line sources, and can utilize 3-d temperature, wind, and turbulence fields.

TRANSIMS (TRANsportation SIMulation System) - a model that simulates traffic flow by following trajectories of multitudes of individual cars. A synthetic population is developed that is statistically similar to the real population in the city of interest and each household is given a daily activities plan (e.g., go from home to work, from work to shopping). On a one second time interval, cars move and interact with each other using cellular automata driving rules. From the simple microscale interactions, complex macroscale traffic behavior develops.

### **Abstracts and Publications**

- Brown, M. and Muller, C. (1997). The effect of microscale urban canyon flow on mesoscale puff dispersion. Amer. Meteorological Society 12th Sympos. on Boundary Layers and Turbulence, Vancouver, B.C.
- Brown, M., Muller, C., and Stretz, P. (1998) Exposure estimates using urban plume dispersion and traffic micro-simulation models. Amer. Meteorological Society 10th Conf. on Air Pollution Meteorology, Phoenix, AZ.
- Brown, M. and Williams, M. (1997).

  The effect of urban canopy
  parameterizations on mesoscale
  meteorological model simulations in
  the Paso del Norte area. American
  Waste Management Association, 90th
  Ann. Conf., Toronto.
- Costigan, Keeley R., Bossert, James E. and Langley, David L. (1998). Simulations of Precipitation Variability over the Upper Rio Grande River Basin. Special Session on Integrated Systems for Observation and Prediction of Flash Flood, River Stage, and Water Resources. American Meteorological Society Ann. Mtg., Phoenix, 13-14 January, 1998.
- Costigan, K. R., Bossert, J. E., Langley, D. L., Turin, H. J., and

- Soll, W. E. (1997). Atmospheric/Hydrologic Models for the Río Grande Basin: Simulations of Precipitation Variability. American Geophysical Union Fall Meeting, December, 1997.
- George, D. (1997). Unstructured 3D Grid Toolbox for Modeling and Simulation, LA-UR-97-3052, to appear in the proceedings of the NASA Ames Device Modeling Workshop, August 7,8, 1997, Santa Clara, CA.
- Jones, E. and K. Olsen. (1997). Three-dimensional finite-difference modeling of non-linear ground motion, to appear in the proceedings of the Northridge Earthquake Research Conference, August 20-22, 1997, Los Angeles.
- Kuprat, A. (1997) Application of Moving Finite Elements to Microstructural Evolution, given at the minisymposium for Moving-Grid Methods for Partial Differential Equations at the SIAM annual meeting in Stanford, CA on July 17, 1997
- Kuprat, A., Cartwright, D., Gammel, J. T., George, D., Kendrick, B., Kilcrease, D., Trease, H. and Walker, R. (1997). X3D Moving Grid Methods for Semiconductor Applications, LA-UR-97-2891, to appear in VLSI Design.
- Soll, W. E., Turin, H. J., Costigan, K.R., and Bossert, J. E. (1997). Atmospheric/Hydrologic Models for the Río Grande Basin: Effects of streamflow on aquifer recharge. American Geophysical Union Fall Meeting, December, 1997.
- Turin, H. J., Gaume, A. N., Bitner, M. J., Hansen, S., and Titus, F. B.. (1997). Albuquerque, New Mexico, USA: A Sunbelt City Rapidly Outgrowing Its Aquifer. International Association of Hydrogeologists, XXVII Congress, Nottingham, UK.

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